Reactivity of Paramagnetic Fe-II-Bis(amidinate) Complexes

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SUPPORTING INFORMATION

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X-ray structure of ^{DippPh}LH:

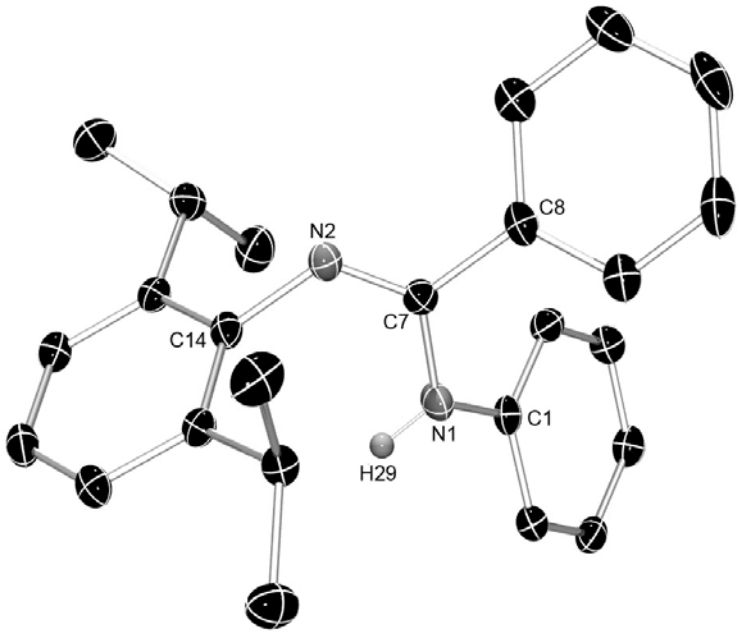

Figure S1. Molecular structure of ^{DippPhL}H (50% probability level). Hydrogen atoms (except NH) removed for clarity.

Table S1. Selected bond distances and angles for ^{DippPh}LH.

Distances [Å]			
N1-C1	1.416(3)	N2-C14	1.425(3)
N1-C7	1.392(3)	C7-C8	1.494(3)
N2-C7	1.281(3)	N1-H29	0.84(2)
Angles [°]			
C1-N1-C7	125.36(18)	N1-C7-N2	124.6(2)
C7-N1-H29	112.3(15)	N1-C7-C8	117.45(18)
C1-N1-H29	117.3(16)	N2-C7-C8	117.64(19)
C7-N2-C14	121.64(17)		

Table S2. Crystal, collection and refinement data for ^{DippPh}LH.

formula	$C_{25}H_{28}N_2$	ρ_{calc} (g/cm^3)	1.168
fw	356.49	θ range (°)	2.68 – 27.39
cryst. dim. (mm)	0.34 x 0.22 x 0.13	λ (Å)	0.71073 (Mo K_α)
colour, habit	l. yellow, block	T (K)	100(1)
crystal system	monoclinic	data collect. time (h)	5.6
space group, no.[53]	$P2_1/c$, 14	no. of meas. refl.	7492
a (Å)	8.2831(7)	no. of unique refl.	4050
b (Å)	23.574(2)	μ (cm^{-1})	0.68
c (Å)	10.735(1)	no. of parameters	356
α (°)	90	weighting scheme: a,b[a]	0.0821, 0.0
β (°)	104.647(2)	$R(F)$ for $F_0 \geq 4\sigma(F_0)$[b]	0.0557
γ (°)	90	$wR(F^2)$[c]	0.1593
Z	4	res. el. dens. (e/Å^3)	–0.28, 0.36(6)
V (Å^3)	2028.1(3)	GoF[d]	1.044

[a] $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, $P = [\max(F_o^2,0) + 2F_c^2] / 3$ [b] $R(F) = \sum (||F_o| - |F_c||) / \sum |F_o|$ [c] $wR(F^2) = [\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]]^{1/2}$ [d] GoF = $[\sum [w(F_o^2 - F_c^2)^2] / (n-p)]^{½}$, n = # refl., p = # param. refined.

Reactions of **1b** with pyridine:

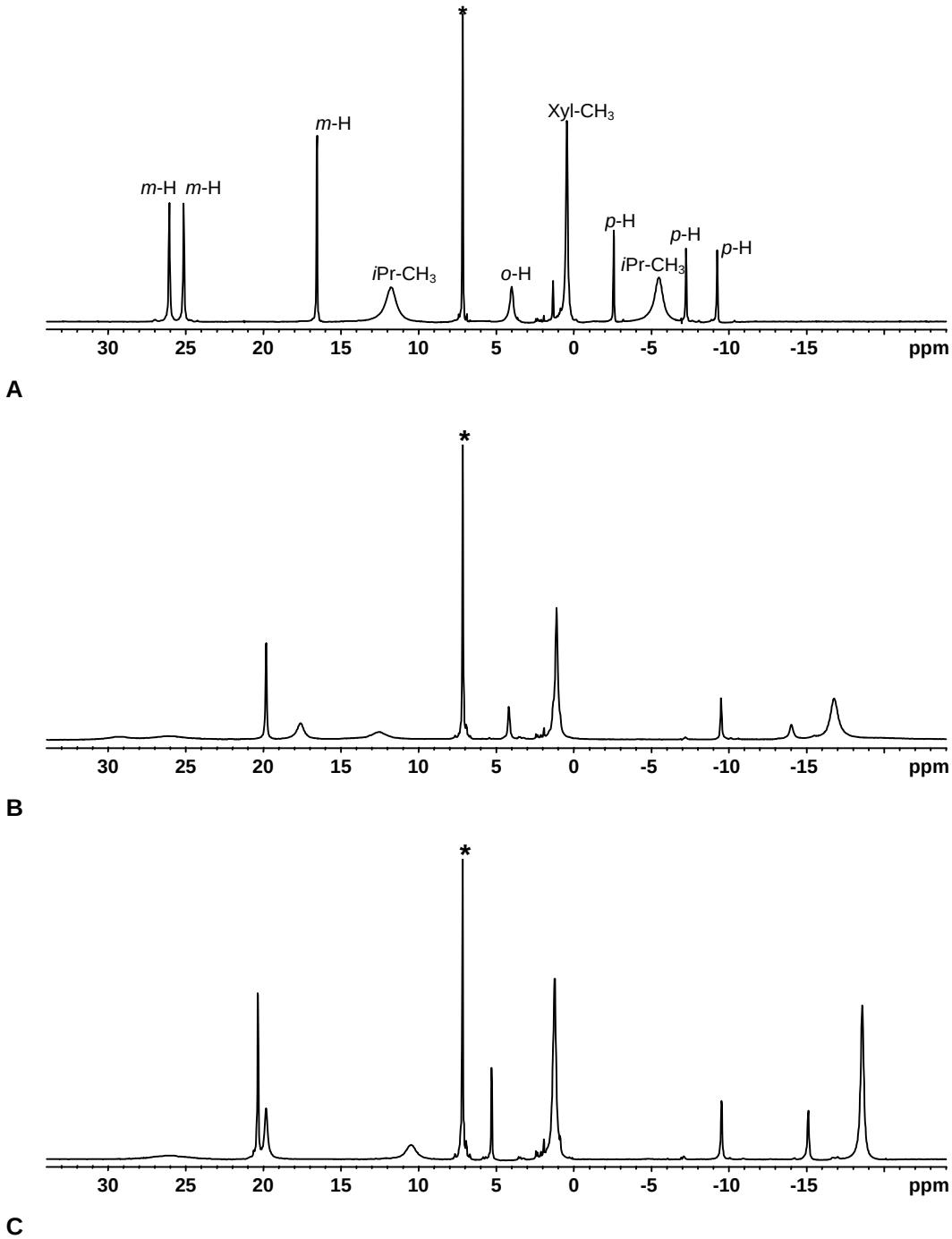

Figure S3. ^{1}H NMR spectra (300 MHz, C_6D_6, 298 K) of **1b** (**A**), **1b** + 1 equiv. py (**B**) and **1b** + 2 equiv. py (**C**)

Magnetic Susceptibility for **1c.bpy**.

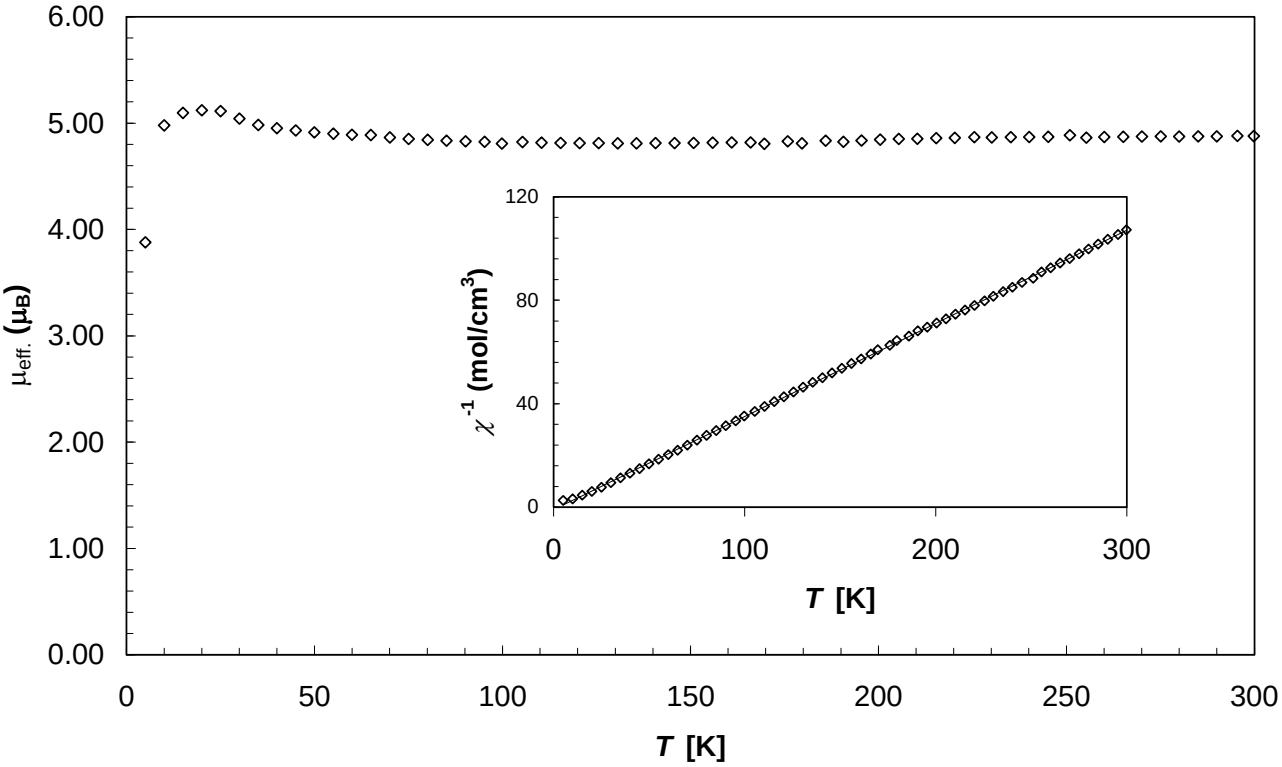

Figure S4. $\mu_{eff.}$ and χ^{-1} for vs T for **1c·bpy**.